Supplementary Information

On the successes and opportunities for discovery of metal oxide photoanodes for solar fuels generators

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Descriptions of contents of the below data tables

p.3-4 **Table S1a-S1b: HiTp composition and photoelectrochemical data for 58 phases measured in our labs**

Table of 58 phases synthesized in combinatorial metal oxide libraries found to be photoactive at 1.23 V vs RHE without addition of sacrificial reagents and without evidence of a photoconductivity or photocorrosion-type response. The resulting assumption is that the OER proceeds under illumination although explicit measurement of evolved O_2 was in general not performed. This table contains additional detail compared to the SI of Ref. 24 (10.1039/C9TA13829C) and is the authoritative table.

id: an index to facilitate indexing across the 2 pages (each page contains the same 58 phases but distinct columns)

standardized_phase_name: Use MP tool to standardize formula units. Explicitly, this is python code str(Composition(fu).reduced_formula).replace(' ','')
where fu is the name of the phase as entered from various sources and Composition is from pymatgen.core.composition

mp_id: The Materials Project id where formula unit and structural match was found

representative_ph: While many phases were tested at multiple pH, only one is shown in this table and is noted by the value in this column. The representative pH was typically chosen as the one where the phase exhibited highest photocurrent under 3.2 eV illumination.

<led>: the wavelength in nm of the LED used for chopped illumination, i.e. one of 385, 455, 515, 600 nm

<type>: The chopped illumination experiments are analyzed to ignore 1 s-scale transients and provide the representative currents: “ill_” and “dark_” for with and without illumination, and “” for the difference between these.

<range>: “unk” for unknown due to lack of some <led> photocurrent, and otherwise indicating range of photon energies (>2.8, 2.4-2.8, 2.1-2.4, <2.1)

Iphoto_<type><led>.uA: The current in µA for each of 3 <type> and 4 <led> values described above.

led_power_<>.mW: The power in mW from an optical power meter calibration near the time of the experiment, from which the photon flux is calculated.

eqe_pct_<led>: The external quantum efficiency in % calculated as the ratio of the e- flux from the Iphoto_<led>.uA and photon flux from led_power_<>.mW. “NA” means measurement was not done, “LOW” means the eqe value was near detectability limit OR there are other reasons to believe the photocurrent isn’t primarily due to OER so the eqe cannot be quantified

onset_<range>: Boolean indicators (“NA” if lacking eqe_pct_<led> info) for range of photon energy where the onset of photoactivity occurs (this is the data used to generate Fig. 3). Onset between X and Y corresponds to no photoactivity at X or lower energy LEDs, and photoactivity at Y and all higher energy LEDs. The detectability limit on eqe_pct is variable due to different illumination intensities, but a conservative threshold of 0.01% is used to determine photoactivity onset. This is a higher threshold than those used in previous works and hence why there are 49 phases instead of 58 in the pie chart.

p. 5 **Table S2: The composition and eqe data used to generate Fig. 4**

The phase list differs from Fig. S1 because Sb (overlap) and Si (substrate signal) are not quantifiable, and eqe and XRF may be measured on different samples than those used in Table S1.

xrf_fu: The difference between the XRF-measured metal fraction of the higher valent cation (determined by the MP oxidation state interpreter) and that of the formula unit, i.e. the x-axis of Fig. 4.

hi_el is element B in Fig. 4 and lo_el is element A, and hi_val and lo_val are the respective nominal valences.

p. 6-21: **Table of 109 metal oxide photoanodes from the literature survey**

The metal oxide phases from the literature follows equivalent criteria as much as possible given different types of experiments and reporting in the literature. The columns of this table are:

phase: formula unit combined with prefix or suffix to distinguish polytypes where necessary. Phase assigned was taken from respective paper and not reassessed in the present work.

Exper gap where available, else theory (eV): The experimentally measured band gap energy (indirect or direct) of the phase, typically from optical spectroscopy in the cited work. See vis_light note below.

reference: shorthand notation for the reference (see below) with first authors surname and 4 digit year. 2 references are listed if information from both papers was required to evaluate our criteria for metal oxide photoanodes.

year: the year from reference, which was used to generate Fig. 1.

mp-id: Materials Project id where formula unit and structure were confirmed.

vis_light: indicator of whether the phase was found to be photoactive with any of the 455,515,600 nm LEDs.

intended to have same meaning as prior table, although per footnote in the main text: “In the literature survey, photoactivity under white light illumination combined with optical identification of a sub-2.8 eV band gap was considered to be sufficient evidence for a visible light photoanode”.

Following the table is a list of the references, some of which do not appear in the table but were useful in assembling the table.

Table S1A: 58 photoanode phases: photon energy onset using 0.01% eqe threshold

id	standardized_phase_name	mp_id	xrf_fu	representative_ph	eqe_pct_385	eqe_pct_455	eqe_pct_515	eqe_pct_600	onset_unk	onset_>2.8	onset_2.4-2.8	onset_2.1-2.4	onset_<2.1
1	FeWO4	mp-19421	-0.131	9	2.016865085	1.517989898	1.397850119	0.08152348	0	NA	0	0	1
2	gamma-V2Cu3O8	mp-504747	-0.068	13	4.860563848	1.240327286	0.249476836	0.021462917	0	NA	0	0	1
3	FeBiO3	mp-24932	-0.114	9	0.404646527	0.152466164	0.087530365	0.018414693	0	NA	0	0	1
4	Y3Fe5O12	mp-19648	-0.047	13	0.892315475	0.388122854	0.155779026	0.011670702	0	NA	0	0	1
5	YMnO3-hex	mp-19227	-0.007	13	0.017602976	0.01523808	0.012992209	0.007380025	0	NA	0	1	0
6	alpha-V2Cu2O7	mp-505508	0.018	7	3.775392214	1.546578	0.316291	0.00723963	0	NA	0	1	0
7	YMn2O5	mp-542867	0.033	10	0.0254	0.0223	0.0127	0.00422	0	NA	0	1	0
8	beta-VAg3O4	mp-19412	0.03	9	0.793574957	0.286847771	0.102714028	LOW	0	NA	0	1	0
9	V2CoO6-tri	mp-622217	-0.031	9	0.10905952	0.072835592	0.068733734	LOW	0	NA	0	1	0
10	VBiO4	mp-504878	0.272	9	2.870632132	0.904765464	0.050991256	LOW	0	NA	0	1	0
11	SrMnO3	mp-568977	0.006	13	0.999494207	0.241125796	0.022047493	LOW	0	NA	0	1	0
12	YFeO3-orth	mp-24999	-0.058	13	0.085457588	0.059637613	0.021107784	LOW	0	NA	0	1	0
13	BaMnO3	mp-19156	0.028	13	0.3736597	0.040066843	0.020271139	LOW	0	NA	0	1	0
14	VFeO4	mp-540630	0.005	9	2.468902041	0.205505876	0.013374769	LOW	0	NA	0	1	0
15	beta-VAgO3	mp-566337	-0.002	9	0.055734787	0.012276275	0.010971497	LOW	0	NA	0	1	0
16	V2Bi4O11	mp-767756	0.085	9	0.489194647	0.144994465	LOW	LOW	0	NA	1	0	0
17	Ca2Mn3O8	mp-18893	-0.083	13	0.337988578	0.102124965	LOW	LOW	0	NA	1	0	0
18	VCrO4-orth	mp-19418	-0.063	9	0.696699527	0.07341557	LOW	LOW	0	NA	1	0	0
19	V4Cr2O13	mp-851269	0.021	9	0.266884776	0.054131306	LOW	LOW	0	NA	1	0	0
20	Ca2MnO4	mp-19050	0.206	10	0.053456058	0.044529912	LOW	LOW	0	NA	1	0	0
21	V2Co3O8	mp-540833	-0.07	9	0.013403011	0.022280778	LOW	LOW	0	NA	1	0	0
22	CaMnO3	mp-19201	0.046	13	0.090752302	0.019139269	LOW	LOW	0	NA	1	0	0
23	V2CoO6-mono	mp-773310	-0.008	9	0.028649638	0.014	LOW	LOW	0	NA	1	0	0
24	V2Ag0.3333O5	none	-0.246	9	0.069562379	0.010008224	LOW	LOW	0	NA	1	0	0
25	Nb10.7V2.38O32.7	none	0.118	9	0.179506169	0.00811969	LOW	LOW	0	1	0	0	0
26	NbVO5	mp-769890	0.063	9	0.703950796	0.006959734	LOW	LOW	0	1	0	0	0
27	V2Ni3O8	mp-542151	-0.003	9	0.006310182	0.00550979	LOW	LOW	0	NA	0	0	0
28	V4.51Pb3.5O14.75	none	-0.017	9	0.006799765	0.003673197	LOW	LOW	0	NA	0	0	0
29	V2ZnO6	mp-551601	-0.006	9	0.066969891	0.001981587	LOW	LOW	0	1	0	0	0
30	YFeO3-hex	mvc-3556	-0.048	13	0.032249	0.001493934	LOW	LOW	0	1	0	0	0
31	V2Pb4O9	mp-647385	0.041	9	0.029849008	0.001449945	LOW	LOW	0	1	0	0	0
32	V(Bi5O8)5	none	0.046	9	0.021661432	0.000966629	LOW	LOW	0	1	0	0	0
33	beta-V2Cu2O7	mp-559660	-0.097	13	4.409481008	NA	NA	NA	1	NA	NA	NA	NA
34	V6Cu11O26	mp-505456	0.075	9	3.305642991	NA	NA	NA	1	NA	NA	NA	NA
35	alpha-V2CuO6	mp-741706	0.021	9	1.842279256	NA	NA	NA	1	NA	NA	NA	NA
36	Zn(FeO2)2	mp-19313	-0.205	10	1.027065296	NA	NA	NA	1	NA	NA	NA	NA
37	V2(CuO2)5	mp-559440	0.039	9	0.362113031	NA	NA	NA	1	NA	NA	NA	NA
38	SrMn3O6	none	-0.042	10	0.259070517	NA	NA	NA	1	NA	NA	NA	NA
39	Mg6MnO8	mp-19239	0.029	10	0.249469197	NA	NA	NA	1	NA	NA	NA	NA
40	Mg2MnO4	none	0.054	10	0.213479035	NA	NA	NA	1	NA	NA	NA	NA
41	CaMn3O6	mp-566229	-0.117	10	0.202796179	NA	NA	NA	1	NA	NA	NA	NA
42	MgMn2O4	mp-32006	0.178	10	0.194687951	NA	NA	NA	1	NA	NA	NA	NA
43	alpha-VAg3O4	mp-18889	0.064	9	0.184164824	LOW	LOW	LOW	0	1	0	0	0
44	V2Zn4O9	mp-504923	-0.039	9	0.133034946	LOW	LOW	LOW	0	1	0	0	0
45	YMnO3-orth	mp-25025	-0.007	13	0.062366836	LOW	LOW	LOW	0	1	0	0	0
46	VCrO4-mono	mp-19688	-0.196	9	0.056721678	NA	NA	NA	1	NA	NA	NA	NA
47	Mn(2/3)Sb(4/3)O4	mp-763546	NA	0	0.037145537	NA	NA	NA	1	NA	NA	NA	NA
48	V2Pb2O7	mp-25796	0.061	9	0.030822376	LOW	LOW	LOW	0	1	0	0	0
49	Mn7SiO12	mp-19650	NA	13	0.025046031	LOW	LOW	LOW	0	1	0	0	0
50	TaVO5	mp-32407	-0.008	9	0.015749702	LOW	LOW	LOW	0	1	0	0	0
51	Ca2V2O7	mp-32434	-0.037	9	0.012806815	NA	NA	NA	1	NA	NA	NA	NA
52	ZrV2O7	mp-565725	-0.005	9	0.009146652	LOW	LOW	LOW	0	NA	0	0	0
53	Fe2WO6	mp-25749	0.04	3	0.008954854	LOW	LOW	LOW	0	NA	0	0	0
54	Mn(Ni3O4)2	mp-19442	-0.035	10	0.006417716	NA	NA	NA	0	NA	NA	NA	NA
55	V2Ni2O7	mp-557404	-0.048	9	0.005874997	LOW	LOW	LOW	0	NA	0	0	0
56	MnGeO3	mp-643577	-0.062	13	0.005325106	NA	NA	NA	0	NA	NA	NA	NA
57	V2Bi8O17	none	0.081	9	0.00432465	NA	NA	NA	0	NA	NA	NA	NA
58	V2Bi12O23	none	0.078	9	0.003472417	LOW	LOW	LOW	0	NA	0	0	0

Table S1b: 58 photoanode phases: source PEC data

id	led_power.mW_385	Iphoto.uA_385	Iphoto_ill.uA_385	Iphoto_dark.uA_385	led_power.mW_455	Iphoto.uA_455	Iphoto_ill.uA_455	Iphoto_dark.uA_455	led_power.mW_515	Iphoto.uA_515	Iphoto_ill.uA_515	Iphoto_dark.uA_515	eqe_pct_600	led_power.mW_600	Iphoto.uA_600	Iphoto_ill.uA_600	Iphoto_dark.uA_600
1	2.81	17.69	17.78	0.08	2.52	14.04	14.12	0.08	0.98	5.70	5.80	0.10	0.08	0.68	0.27	0.36	0.09
2	3.76	56.75	56.75	0.00	2.47	11.24	11.16	-0.09	1.16	1.24	1.16	-0.07	0.02	2.46	0.26	0.35	0.08
3	2.81	3.55	3.76	0.21	2.52	1.41	1.68	0.27	0.98	0.36	0.56	0.21	0.02	0.68	0.06	0.24	0.18
4	2.14	5.96	5.82	-0.14	1.90	2.71	2.70	-0.01	0.79	0.51	0.54	0.03	0.01	0.50	0.03	0.11	0.08
5	2.14	0.12	0.14	0.01	1.90	0.11	0.11	0.00	0.79	0.04	0.07	0.03	0.01	0.50	0.02	0.05	0.04
6	2.79	32.76	33.45	0.71	1.33	7.55	7.68	0.15	0.62	0.84	0.84	-0.03	0.01	1.33	0.05	0.12	0.08
7	2.14	0.17	0.12	-0.05	2.00	0.16	0.11	-0.06	0.80	0.04	0.05	0.01	0.00	0.50	0.01	0.03	0.02
8	2.96	7.29	16.18	8.80	2.37	2.47	8.76	6.13	0.96	0.41	0.45	0.02	LOW	0.80	0.04	4.42	4.30
9	2.96	1.00	1.06	-0.10	2.37	0.63	0.43	-0.20	0.96	0.27	0.23	-0.04	LOW	0.80	4.58	3.52	-1.00
10	2.96	26.39	26.45	0.06	2.37	7.80	9.02	1.19	0.96	0.20	1.10	0.88	LOW	0.80	0.00	0.81	0.83
11	2.96	9.23	12.78	2.99	2.37	2.08	3.39	1.20	0.96	0.09	0.70	0.56	LOW	0.80	0.00	0.45	0.43
12	2.14	0.57	0.69	0.11	1.90	0.42	0.50	0.08	0.79	0.07	0.15	0.09	LOW	0.50	0.00	0.08	0.08
13	2.96	3.45	2.66	-0.78	2.37	0.35	2.31	1.83	0.96	0.08	0.04	-0.03	LOW	0.80	0.02	0.92	0.87
14	2.96	22.69	22.69	0.00	2.37	1.77	1.88	0.09	0.96	0.05	-0.14	-0.20	LOW	0.80	0.00	0.00	0.01
15	2.96	0.51	10.66	10.18	2.37	0.11	3.26	3.06	0.96	0.04	2.13	2.00	LOW	0.80	0.03	1.42	1.36
16	2.96	4.50	4.49	-0.01	2.37	1.25	1.39	0.14	0.96	0.01	0.10	0.09	LOW	0.80	0.00	0.07	0.07
17	2.14	2.26	2.41	0.13	1.90	0.71	0.82	0.09	0.79	0.07	0.09	0.03	LOW	0.50	0.00	0.10	0.09
18	2.96	6.40	6.36	-0.04	2.37	0.63	1.37	0.73	0.96	0.04	0.61	0.57	LOW	0.80	0.08	0.62	0.55
19	2.96	2.45	3.60	1.14	2.37	0.47	2.47	1.91	0.96	0.01	1.88	1.85	LOW	0.80	0.00	1.80	1.81
20	2.20	0.37	2.59	2.19	2.10	0.34	2.02	1.66	0.70	0.12	1.67	1.55	LOW	0.44	0.05	1.33	1.26
21	2.96	0.12	0.15	0.02	2.37	0.19	-0.32	-0.62	0.96	0.00	0.09	0.12	LOW	0.80	0.00	0.12	0.12
22	2.96	0.84	5.42	4.00	2.37	0.17	1.78	1.46	0.96	0.05	1.24	1.17	LOW	0.80	-0.01	0.84	0.85
23	2.96	0.26	0.86	0.57	2.37	0.09	0.13	0.04	0.96	0.00	0.20	0.18	LOW	0.80	0.00	0.25	0.25
24	2.70	0.59	0.73	0.13	2.70	0.10	0.18	0.07	1.10	0.00	0.11	0.11	LOW	0.81	0.03	0.15	0.13
25	2.96	1.65	1.90	0.25	2.37	0.07	0.74	0.67	0.96	0.00	0.58	0.57	LOW	0.80	0.00	0.57	0.57
26	2.96	6.47	6.75	0.28	2.37	0.06	0.25	0.19	0.96	0.01	0.16	0.14	LOW	0.80	0.01	0.14	0.13
27	2.96	0.06	0.03	-0.03	2.37	0.05	0.11	0.05	0.96	0.02	-0.16	-0.19	LOW	0.80	-0.01	-0.14	-0.13
28	2.96	0.06	0.06	0.00	2.37	0.03	0.15	0.12	0.96	0.00	0.11	0.11	LOW	0.80	0.00	0.10	0.10
29	2.96	0.62	0.60	-0.02	2.37	0.02	-0.02	-0.04	0.96	0.00	-0.04	-0.03	LOW	0.80	0.00	-0.03	-0.03
30	2.14	0.22	0.10	-0.11	1.90	0.01	0.23	0.21	0.79	0.00	0.19	0.18	LOW	0.50	0.00	0.17	0.17
31	2.96	0.27	0.23	-0.04	2.37	0.01	-0.03	-0.04	0.96	0.00	-0.04	-0.04	LOW	0.80	0.00	-0.04	-0.04
32	2.96	0.20	0.17	-0.02	2.37	0.01	-0.02	-0.03	0.96	0.00	-0.03	-0.03	LOW	0.80	0.00	-0.04	-0.04
33	3.76	51.48	51.49	0.01	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.01
34	2.96	30.38	30.28	-0.11	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
35	2.96	16.93	16.96	0.03	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
36	1.65	5.26	5.17	-0.09	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
37	2.96	3.33	3.32	-0.01	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
38	2.60	2.10	2.21	0.10	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
39	2.60	2.02	1.25	-0.75	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
40	2.60	1.73	1.04	-0.69	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
41	2.96	1.86	1.18	-0.68	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
42	2.60	1.58	0.92	-0.66	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
43	2.96	1.69	2.41	0.67	2.37	-0.16	0.01	0.16	0.96	0.03	0.17	0.14	LOW	0.80	0.04	0.16	0.12
44	2.96	1.22	1.26	0.03	2.37	0.00	-0.04	-0.04	0.96	0.00	-0.05	-0.05	LOW	0.80	0.00	-0.05	-0.05
45	2.96	0.58	0.18	-0.34	2.70	0.11	0.29	0.17	1.10	0.04	0.40	0.35	LOW	0.81	0.04	0.39	0.34
46	2.96	0.52	1.63	0.97	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
47	4.10	0.47	0.97	0.44	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
48	2.96	0.28	0.18	-0.14	2.37	0.03	0.13	0.10	0.96	0.01	0.12	0.11	LOW	0.80	0.00	0.14	0.14
49	2.96	0.23	0.74	0.51	2.70	0.00	0.55	0.54	1.10	0.01	0.31	0.30	LOW	0.81	0.01	0.16	0.17
50	2.96	0.15	0.15	0.00	2.37	0.01	0.16	0.14	0.96	0.01	0.12	0.11	LOW	0.80	0.01	0.07	0.06
51	3.25	0.13	0.21	0.10	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
52	2.96	0.08	0.08	-0.01	2.37	0.00	0.01	0.00	0.96	0.00	-0.01	-0.01	LOW	0.80	0.00	-0.01	-0.01
53	2.40	0.07	0.25	0.17	1.80	0.00	0.16	0.16	0.77	0.00	0.15	0.15	LOW	0.54	0.01	0.23	0.22
54	2.60	0.05	0.09	0.07	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
55	2.96	0.05	0.12	0.06	2.37	0.03	0.11	0.09	0.96	0.01	0.02	0.01	LOW	0.80	0.00	0.11	0.12
56	2.96	0.05	0.04	-0.01	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
57	2.96	0.04	0.06	0.03	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
58	2.96	0.03	0.09	0.08	2.37	0.00	-0.05	-0.04	0.96	0.00	-0.04	-0.04	LOW	0.80	0.00	-0.05	-0.05

Table S2: EQE and composition differences for 56 photoanode phases

standardized_phase_name	mp_id	hi_el	hi_val	lo_el	lo_val	xrf_fu	eqe_pct_385	eqe_pct_455	eqe_pct_515	eqe_pct_600
BaMnO3	mp-19156	Mn	4	Ba	2	0.028	0.3736597	0.040066843	0.020062166	0.006211212
Ca2Mn3O8	mp-18893	Mn	4	Ca	2	-0.083	0.337988578	0.102124965	0.020507299	-0.001716283
Ca2MnO4	mp-19050	Mn	4	Ca	2	0.206	0.053456058	0.044529912	0.041987133	0.022623697
Ca2V2O7	mp-32434	V	5	Ca	2	-0.037	0.012806815			
CaMn3O6	mp-566229	Mn	3.33	Ca	2	-0.117	0.202796179			
CaMnO3	mp-19201	Mn	4	Ca	2	0.046	0.090752302	0.019139269	0.011911911	-0.001606348
Fe2WO6	mp-25749	W	6	Fe	3	0.04	0.008954854	-0.001710599	0.001172464	0.002855726
FeBiO3	mp-24932	Fe	3	Bi	3	-0.114	0.404646527	0.130344513	0.044439436	0.005552666
FeWO4	mp-19421	W	6	Fe	2	-0.131	2.016865085	1.517989898	1.397850119	0.08152348
Mg2MnO4	none	Mn	4	Mg	2	0.054	0.213479035			
Mg6MnO8	mp-19239	Mn	4	Mg	2	0.029	0.249469197			
MgMn2O4	mp-32006	Mn	3	Mg	2	0.178	0.194687951			
Mn(Ni3O4)2	mp-19442	Ni	2.33	Mn	2	-0.035	0.006417716			
MnGeO3	mp-643577	Ge	4	Mn	2	-0.062	0.005325106			
Nb10.7V2.38O32.7	none	Nb	5	V	5	0.118	0.179506169	0.001449945	0.001253875	0.000107093
NbVO5	mp-769890	Nb	5	V	5	0.063	0.703950796	0.002706559	0.003030215	0.003533961
SrMn3O6	none	Mn	3.33	Sr	2	-0.042	0.259070517			
SrMnO3	mp-568977	Mn	4	Sr	2	0.006	0.999494207	0.241125796	0.022047493	0.000642538
TaVO5	mp-32407	Ta	5	V	5	-0.008	0.015749702	0.001546604	0.001567357	0.001285077
V(Bi5O8)5	none	V	5	Bi	3	0.046	0.021661432		0.000940414	-0.00042836
V2(CuO2)5	mp-559440	V	5	Cu	2	0.039	0.362113031			
V2Ag0.3333O5	none	V	4.83	Ag	1	-0.246	0.085372011	0.012924527	0.001289711	0.013652256
V2Bi12O23	none	V	5	Bi	3	0.078	0.003472417	-0.000338321	0.000313471	0.00021418
V2Bi4O11	mp-767756	V	5	Bi	3	0.085	0.489194647	0.144994465	0.001880831	-0.00042836
V2Bi8O17	none	V	5	Bi	3	0.081	0.00432465			
V2Co3O8	mp-540833	V	5	Co	2	-0.07	0.013403011	0.022280778	-0.000835925	0.000856719
V2CoO6-tri	mp-622217	V	5	Co	2	-0.031	0.10905952	0.072835592	0.068733734	1.177022191
V2CoO6-mono	mp-773310	V	5	Co	2	-0.008	0.028649638		0.000835923	0.000321269
alpha-V2Cu2O7	mp-505508	V	5	Cu	2	0.018	3.775392214			0.00723963
beta-V2Cu2O7	mp-559660	V	5	Cu	2	-0.097	4.409481008			2.537590739
gamma-V2Cu3O8	mp-504747	V	5	Cu	2	-0.068	4.860563848	1.240327286	0.249476836	0.021462917
alpha-V2CuO6	mp-741706	V	5	Cu	2	0.021	1.842279256			
V2Ni2O7	mp-557404	V	5	Ni	2	-0.048	0.005874997	0.003576526	0.002507771	0.001070898
V2Ni3O8	mp-542151	V	5	Ni	2	-0.003	0.006310182	0.00550979	0.004911043	-0.002034703
V2Pb2O7	mp-25796	V	5	Pb	2	0.061	0.030822376	0.003189878	0.001253885	0.000963807
V2Pb4O9	mp-647385	V	5	Pb	2	0.041	0.029849008	0.001449945	0.000731434	0.000321269
V2Zn4O9	mp-504923	V	5	Zn	2	-0.039	0.133034946	9.67E-05	-0.000208981	-0.000749629
V2ZnO6	mp-551601	V	5	Zn	2	-0.006	0.066969891	0.001981587	-0.001149394	-3.04E-10
V4.51Pb3.5O14.75	none	V	4.67	Pb	2	-0.017	0.006799765	0.003673197	0.000940414	0.000535448
V4Cr2O13	mp-851269	V	5	Cr	3	0.021	0.266884776	0.054131306	0.001671858	-0.000214177
V6Cu11O26	mp-505456	V	5	Cu	2	0.075	3.305642991			
alpha-VAg3O4	mp-18889	V	5	Ag	1	0.064	0.184164824	-0.018075938	0.007000868	0.01070898
beta-VAg3O4	mp-19412	V	5	Ag	1	0.03	0.793574957	0.286847771	0.102714028	0.011351544
beta-VAgO3	mp-566337	V	5	Ag	1	-0.002		0.012276275	0.010971497	0.007710434
VBiO4	mp-504878	V	5	Bi	3	0.272	2.870632132	0.904765464	0.050991256	-0.000642541
VCrO4-orth	mp-19418	V	5	Cr	3	-0.063	0.696699527	0.07341557	0.010449053	0.019276149
VCrO4-mono	mp-19688	V	5	Cr	3	-0.196	0.056721678			
VFeO4	mp-540630	V	5	Fe	3	0.005	2.468902041	0.205505876	0.013374769	-0.00042836
Y3Fe5O12	mp-19648	Y	3	Fe	3	-0.047	0.892315475	0.388122854	0.155779026	0.011670702
YFeO3-orth	mp-24999	Y	3	Fe	3	-0.058	0.085457588	0.059637613	0.021107784	0.001029769
YFeO3-hex	mvc-3556	Y	3	Fe	3	-0.048	0.00274462	0.001493934	0.000764245	0.000171634
YMn2O5	mp-542867	Mn	3.5	Y	3	0.033	0.006549673			
YMnO3-hex	mp-19227	Y	3	Mn	3	-0.007	0.017602976	0.01523808	0.012992209	0.007380025
YMnO3-orth	mp-25025	Y	3	Mn	3	-0.007	0.062366836			
Zn(FeO2)2	mp-19313	Fe	3	Zn	2	-0.205	1.027065296			
ZrV2O7	mp-565725	V	5	Zr	4	-0.005	0.009146652	0.000434983	-0.000417963	0.000321269

Table S3: 109 metal oxide photoanode phases

Phase	Exper gap where available, else theory (eV)	reference	year	mp-id	vis_light
TiO2	3.2	Fujishima1972	1972	mp-2657	0
SrTiO3	3.2	Mavroides1975	1975	mp-5229	0
WO3	3.2	Hodes1976	1976	mp-619461	0
alpha-Fe2O3	1.9	Hardee1976	1976	mp-24972	1
Fe2WO6	1.5	Leiva1982	1982	mp-25749	1
TiNiO3		deKorte1982	1982	mp-18732	0
Nb2NiO6	>3	deKorte1982	1982	mp-608621	0
CuWO4	2.34	Doumerc 1984	1984	mp-510632	1
MgTiO3	3.7	deHaart1984	1984	mp-3771	0
Nb2ZnO6	4	Kudo1999_overall	1999	mp-17177	0
K2La2Ti3O10	3.4-3.5	Domen2000	2000	mp-6548	0
Rb2La2Ti3O10	3.4-3.5	Domen2000	2000	none	0
K4Nb6O17	3.3	Domen2000	2000	mp-560692	0
Sr2Nb2O7	3.9	Kudo2000	2000	uncertain	0
Sr2Ta2O7	4.6	Kudo2000	2000	uncertain	0
RbNdTa2O7	3.9	Machida2000	2000	none	0
LiTaO3	4.7	Kato2001	2001	mp-1105280	0
NaTaO3	4	Kato2001	2001	mp-3858	0
KTaO3	3.6	Kato2001	2001	mp-3614	0
VBiO4	2.4	Sayama2003	2003	mp-504878	1
La2Ti2O7	3.82	Hwang2003	2003	mp-559768	0
Pr2Ti2O7	2.99	Hwang2003	2003	mp-15201	1
LaPrTi2O7	2.98	Hwang2003	2003	mp-559768	1
Nd2Ti2O7	3.65	Hwang2003	2003	mp-15201	0
LaNdTi2O7	3.68	Hwang2003	2003	none	0
BaZn1/3Nb2/3O3	3.9	Yin2004	2004	mp-12193	0
VCu2BiO6	2.1	Liu2005	2005	mp-699707	1
VZn2BiO6	2.4	Liu2006	2006	none	1
VFeO4	2	Arai2007	2007	mp-540630	1
FeBiO3	2.1	Chen2007_APL	2007	mp-24932	1
YBiWO6	2.71	Liu2008	2008	none	1
Bi2MoO6	2.64	Yu2008	2008	mp-25708	1
VInO4	3.2	Enache2009, Krol2011	2009	mp-25113	0
Bi2WO6	2.7	Zhang2009	2009	mp-25730	1
TlVO4	2.94	Butcher2010	2010	none	1
Cd2SnO4-cub	2.5	Kelkar2012	2012	mp-1104726	1
Cd2SnO4-ortho	2.5	Kelkar2012	2012	mp-5966	1
TiFe2O5	2.2	Courtin2014	2014	mp-763506	1
alpha-V2CuO6	1.95	Guo2015	2015	mp-741706	1
beta-V2Cu3O8	2.05	Seabold2015	2015	mp-600273	1
V4Fe2O13	2.25	Tang2015	2015	mp-565529	1
alpha-V2Cu2O7	2	Zhou2015	2015	mp-505508	1
beta-V2Cu2O7	2	Zhou2015	2015	mp-559660	1
gamma-V2Cu3O8	2	Zhou2015	2015	mp-504747	1
V6Cu11O26	2	Zhou2015	2015	mp-505456	1
V2NiO6	2.16	Dang2015	2015	mp-32382	1
alpha-VAg3O4	2.2	Chemelewski2015	2015	mp-18889	1
Zn(FeO2)2	1.9-2.1	Kim2015	2015	mp-19313	1
Fe2CoO4	1.36	Helaili2015	2015	mp-1103499	1
Fe2CuO4	1.37	Helaili2015	2015	mp-770107	1
V2Bi4O11	2.15	Jiang2016	2016	mp-767756	1
V2FeO4	1.9	Mandal2016	2016	mp-510496	1
CaTi4(CuO4)3	1.5	Kushwaha2016	2016	mp-647452	1
LaFeO3	2.07	Peng2016	2016	mp-542920	1

Ca(BiO2)2		Wang2017	2017	mp-558751	0
Ca(Bi3O5)2	2.3	Liu2017	2017	none	1
V4Cr2O13	2.3	Yan2017	2017	mp-851269	1
VCrO4-orth	2.38	Yan2017	2017	mp-19418	1
VCrO4-mono	2.27	Yan2017	2017	mp-17831	1
V2CoO6-mono	2.25	Yan2017	2017	mp-773310	1
V2Co3O8	2.22	Yan2017	2017	mp-540833	1
V2Ni2O7	2.5	Yan2017	2017	mp-557404	1
V2Ni3O8	2.5	Yan2017	2017	mp-542151	1
beta-VAg3O4	2.35	Yan2017	2017	mp-19412	1
SrMnO3	1.66	Shinde2017	2017	mp-568977	1
MgMn2O4	2.08	Shinde2017	2017	mp-32006	1
Mn(Ni3O4)2	2.1	Shinde2017	2017	mp-19442	1
BaMnO3	2.16	Shinde2017	2017	mp-19156	1
Ca2Mn3O8	2.4	Shinde2017	2017	mp-18893	1
MgTi2O5	3.4	Ehsan2017	2017	mp-28232	0
Nb4Pb3O13	2.9	Tian2017	2017	none	1
YFeO3-hex	1.88	Guo2017	2017	mvc-3556	1
FeWO4	1.8	Zhou2018	2018	mp-19421	1
alpha-SnWO4	1.9	Ko?lbach2018	2018	mp-19654	1
V2(CuO2)5		Jiang2018	2018	mp-559440	1
Ni3Mn3Ti6O18	1.7	Munawar2019	2019	none	1
Nb2Sn2O7	2.3	Liu2019	2019	mp-556524	1
YVO4	3.2	Lan2019	2019	mp-19133	0
SnNb2O6	2.4	Matsuo2019	2019	mp-3324	1
Mg2MnO4		Noh2019	2019	none	0
CaMn3O6		Zhou2019	2019	mp-566229	0
MnGeO3		Zhou2019	2019	mp-643577	0
Mg6MnO8		Zhou2019	2019	mp-19239	0
Mn(2/3)Sb(4/3)O4		Zhou2019	2019	mp-763546	0
Mn7SiO12	1.9	Zhou2019	2019	mp-19650	0
SrMn3O6		Zhou2019	2019	none	0
Nb10.7V2.38O32.7	2.4	Zhou2019	2019	none	1
V2Ag0.3333O5	2.5	Zhou2019	2019	none	1
Ca2V2O7		Zhou2019	2019	mp-32434	0
V2CoO6-tri	2.4	Zhou2019	2019	mp-622217	1
V2Pb2O7		Zhou2019	2019	mp-25796	0
V2Pb4O9	2.4	Zhou2019	2019	mp-647385	1
V2Zn4O9		Zhou2019	2019	mp-504923	0
V2ZnO6	2.4	Zhou2019	2019	mp-551601	1
ZrV2O7		Zhou2019	2019	mp-565725	0
V4.51Pb3.5O14.75	2.4	Zhou2019	2019	none	1
V(Bi5O8)5	2.4	Zhou2019	2019	none	1
NbVO5	2.4	Zhou2019	2019	mp-769890	1
TaVO5		Zhou2019	2019	mp-32407	0
Y3Fe5O12	2.4	Zhou2019	2019	mp-19648	1
YFeO3-orth	2.4	Zhou2019	2019	mp-24999	1
YMn2O5	2.5	Zhou2019	2019	mp-542867	1
YMnO3-hex	2.4	Zhou2019	2019	mp-19227	1
YMnO3-orth	2.3	Zhou2019	2019	mp-25025	0
CaMnO3	1.41	Zhou2019	2019	mp-19201	1
beta-VAgO3	2.4	Zhou2019	2019	mp-566337	1
Ca2MnO4	1.79	Zhou2019	2019	mp-19050	1
V2Bi8O17		Zhou2019	2019	none	0
V2Bi12O23	2.3	Zhou2019	2019	none	0

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